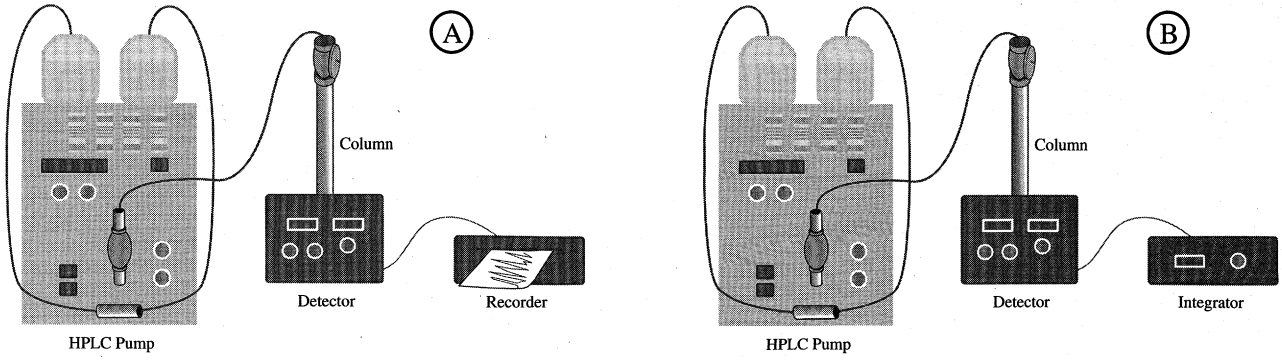


Schematics for five possible types of chromatographic data systems available in the 1990s are shown above and on pages 183 and 184: A–Strip-chart recorder data system; B–Integrator-data system; C–Integrator-PC interface data system (page 183); D–PC-based direct data system (page 183); and E–Minicomputer-based direct data systems (page 184).

Chromatography data systems for lipid analysis

For quantitative lipid analysis, there are currently several separation methodologies available, including gas–liquid chromatography (GC or GLC), high-performance liquid chromatography (HPLC), supercritical fluid chromatography (SFC), and capillary electrophoresis (CE or CZE). Each of these techniques generates data that must be recorded, integrated, and manipulated in a variety of ways. In the 1990s there are currently a number of tools available to assist in the acquisition and handling of chromatographic data. This article will describe and compare some advantages and disadvantages of these various tools.

History of chromatography data systems

The first gas–liquid chromatographs were pioneered in the 1960s and used strip chart recorders for data acquisition. Recorders have improved in quality and decreased in size and maintenance requirements since those of the 1960s. The invention of electronic integrators permitted the printout of both the chromatogram and peak areas of interest. The first integrators became commercially available in the 1970s. The Hewlett Packard model 3390 series and the Thermo-Separations (formerly Spectra-Physics) model 4270 series have been the most popular integrators of all time, and both continue to be marketed and widely used today.

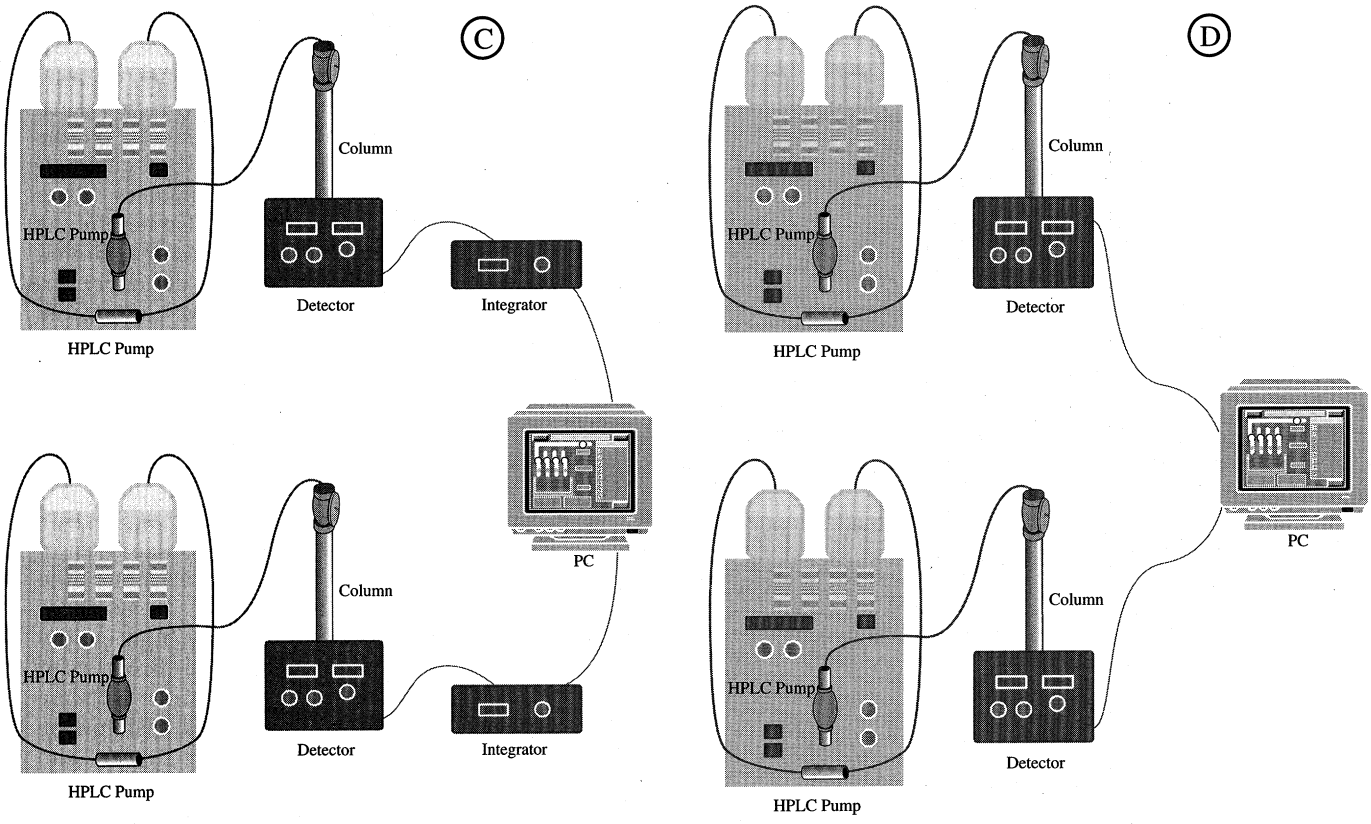
The appearance of the first Apple and IBM personal computers (PC) in the early 1980s paved the way for the development of PC data acquisition systems. As PCs have become more powerful and more popular, a number of PC-based chromatography data systems have coevolved and have become more sophisticated and more popular.

Comparison of the features

There are five basic types of chromatography data systems available in the 1990s, and the configurations of these five types of systems are compared (Figure A, B, C, D, and E).

Strip chart recorders are the simplest type of chromatographic data system and require the least maintenance. Recorders can be used for qualitative analysis and for quantitative analysis, if the peak areas are quantified with a planimeter, or by some form of triangulation or digitization. Alternatively, peak area can be estimated quite accurately using the "cut-and-weigh" technique, which involves cutting peaks from the chart paper with scissors and weighing them on an accurate analytical balance.

Integrators are still used widely in the 1990s and, because of their reliability, accuracy and ease of use, are very appropriate for many applications. Integrators print out the chromatogram, calculate peak areas with predetermined parameters, and also can calculate masses. A major disadvantage of integrators is that the chromatographer must usually select integration parameters, such as peak width, area reject, threshold, and output mV scale values, before the sample is analyzed. If, after the sample is analyzed, the chromatographer finds that one or more of these parameters were not optimal, then the parameters must be changed and the sample reinjected. Some modern integrators have sufficient memory to store one or two chromatograms—allowing some parameters to be reset

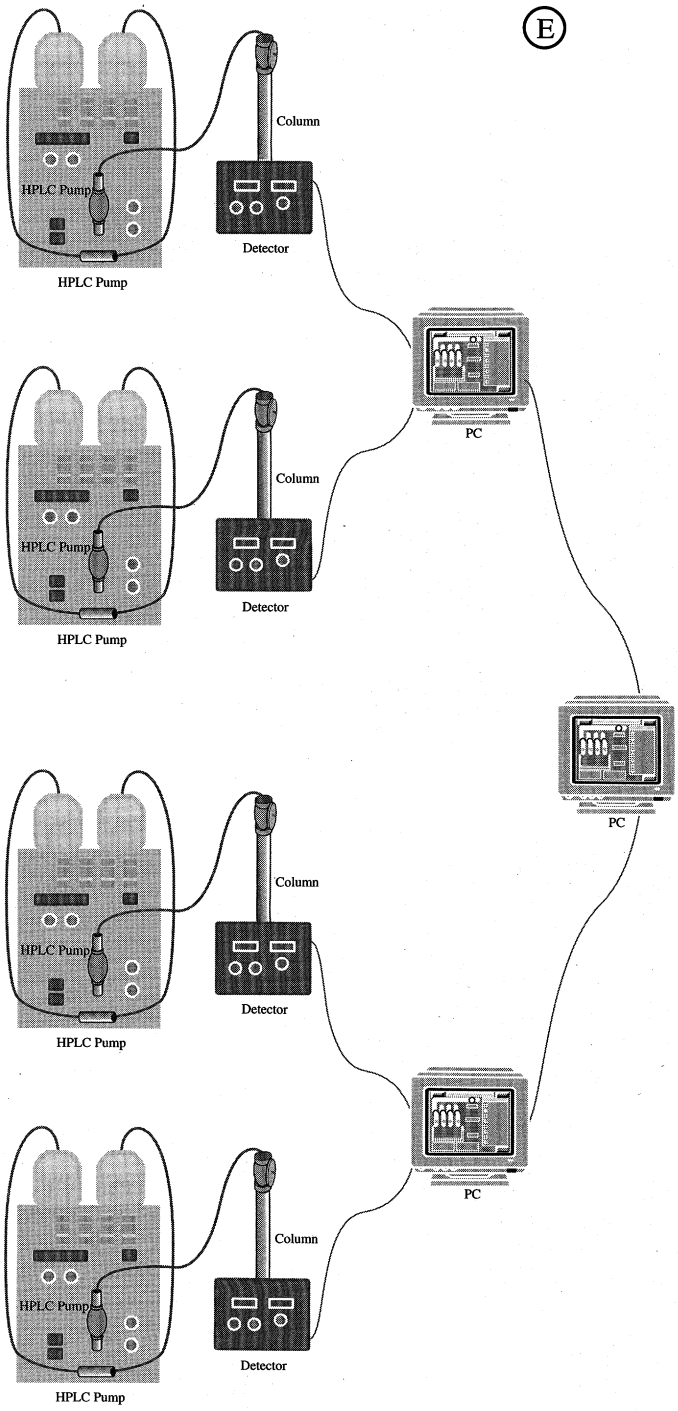


and recalculated, but this has to be done soon after an analysis or the file is written over.

For laboratories that perform multiple lipid analyses and need to, or would like to, electronically store, integrate, and report chromatographic data, the selection of options becomes more complex. The simplest option in this field, for a laboratory that is now using integrators and would like to store data electronically, is to purchase integrator–PC interface software. This type of product literally connects the integrator to a PC and stores all of the data fed into the integrator on the hard drive of the PC. The main advantage of this type of system is that a large amount of data can be stored in the PC, and the data can be retrieved any time, integrated using a variety of automatic or manual integration parameters, and printed in a variety of formats. The abovementioned problem concerning the inability of most integrators to print out data in more than one predetermined set of parameters is overcome with the integrator–PC-based chromatography system. With an integrator–PC interface software system, chromatographic raw data can be recalled, reintegrated until the optimal integration parameters are determined, and reprinted until the optimum x-axis (mV detector output) and y-axis (time) values are found.

Another advantage of this and other computer-based chromatography systems is the ability to archive data both electronically and in standard 8.5 x 11" paper, which can be conveniently stored. The ability to readily archive data is especially important for labs that need to comply with GLP (Good Laboratory Practice) standards. Many older integrators used thermal paper, which often had to be taped into a notebook and whose print quality often deteriorated over time. A disadvantage of the integrator–PC interface system is that it requires the purchase of a separate integrator for each detector. Another disadvantage of some of the products in this category is that they are not multitasking; when stored data is recalled from the PC hard disk, it must be fed back into the integrator (when it is not collecting data) for reintegration and reporting. However, this limitation does not apply to the products of other vendors in this category, where the chromatographer can process data directly from the PC and print it out with a dot-matrix, ink-jet, or laser printer.

A chromatographic data system that has all of the advantages of an integrator–PC interface system is a PC-based direct chromatographic data system, which functions without the need of an integrator(s). There are two ways to connect the direct PC systems. Some have interface cards (usually a board that fits into a PC expansion slot) which are connected directly to the detector(s). Others, like PE Nelson TurboChrom, use an interface box. The analog signal lines are connected to the interface box. The analog signal is digitized in the interface box and sent to the PC *via* a computer communica-



Minicomputer-based direct data systems

tions line. The interface box allows the analog signal lines to be shorter and less likely to pickup any electronic noise. These same interface boxes are used in some minicomputer-based data systems.

PC-based chromatography data systems are often more expensive than integrator–PC interface systems, but because they do not require the purchase of integrators, the cost may be comparable, or may even be less expensive, for systems with multiple detectors. These systems are available for both IBM-compatible and Macintosh computers. Some of these systems may also require the purchase of external analog to digital converters for use with certain detectors. Most of the IBM-compatible systems run in a Windows environment, but some use MS-DOS or OS/2. A major advantage of most of the products in this category is that they are multitasking, meaning that data can be manipulated in the PC while chromatographic separation data are still being collected. Most of the products in this category also drive laser printers, so the chromatograms are of very high quality and often can be used directly for publication. In addition, the software often allows editing and customizing of chromatograms for reports and publications by removing retention times and/or adding various labels. A potential disadvantage of this type of software is that the number of HPLC systems and detectors that can be connected to the system (often limited to a maximum of 4 or 16 detectors) may not be enough for larger analytical laboratories. Some laboratories have reported success in creating a "peer-to-peer local area network" using PC workstations, each running with MS Windows for Workgroups (1).

For even larger laboratories, the solution may be a minicomputer-based software system (available from such vendors as Beckman, Fisons, Hewlett Packard, PE Nelson, Perkin-Elmer, and Waters) that can handle more HPLC systems and detectors and can often function as part of a total laboratory information management system. Sometimes a series of PC-based chromatography workstations can be linked to a minicomputer for centralized storage of data.

Another type of specialized chromatography data system that also

should be mentioned is one designed to handle the data from a diode-array detector, or other types of detectors that output data on multiple channels simultaneously. The data generated from LC–MS (liquid chromatography–mass spectrometry) instruments often also require specialized software. The software for these types of chromatographic systems is often only available from the vendors of these detectors. Because these types of detection systems generate a large amount of data per analysis, it is probably wise to make sure that a PC used with these types of chromatography data systems contains a very large hard disk to store as much data as possible.

Comparison of data acquisition systems vs. data and control systems

There are two basic types of chromatography software systems on the market today. One type only has data acquisition capability and its only connections to the HPLC or other chromatographic systems are the output of the detector(s) and sometimes a start/stop relay connected to the injector or autosampler (autoinjector). The second type of software contains data acquisition capability, but it also contains the information to control and "run" the various components of the chromatographic system. The latter type of software is commonly obtained as part of a "turnkey system" from most of the major vendors [including, but not limited to, such companies as Autochrome, Beckman, Dionex, Gilson, Hewlett Packard, Hitachi, ISCO, Perkin Elmer, Shimatsu, Thermo-Separations (formerly Spectra Physics), Varian, and Waters].

In contrast, the "data acquisition system only" software is usually obtained from "third party" vendors (including, but not limited to, such products as ChromPerfect from Justice Innovations, EZ-Chrom FrontRunner from Scientific Software Inc., Intuitive Chromatography from Borwin, and Turbochrom from PE Nelson) and is capable of handling the output signals from a variety of detectors. When used with an autosampler, both types of software can be used to construct a fully automated chromatography system. However, with the "data acquisition system only" software, a modern programmable autosampler must be used to control the starting and stopping of other chromatography components and the software.

Approximate costs

Strip chart recorders are the least expensive chromatography data system and range in price from less than $1,000 to $2,500. Integrators range in cost from $1,700–4,000, with such extra-cost options as dual channel capability. Integrator–PC interface software packages can be added to the lab that already has an integrator(s) and an appropriate PC for as little as $500. PC-based chromatography data systems start at $4,000, which often includes the price of a PC. Prices for multiple-chromatograph and multiple-detector systems increase accordingly, as do the prices for minicomputer-based multiple input systems.

Chromatography systems of the future

As computer and microprocessor technology continue to progress, it is inevitable that chromatography software also will continue to improve and to evolve. Most of the chromatography software vendors are continually upgrading their products so that they can take advantages of the faster

and more advanced PCs and microcomputers that are continually being introduced. As network technology has become more advanced, it is now technically possible for a lipid analyst to monitor and control chromatographic instruments from remote terminals in another part of the building, from his/her home, and from any conceivable networked or modem-accessible location in the world. A recent article describes the hardware and software which can be used to monitor activity in the laboratory from home or on the road (2). In the future, this level of convenience will become more easily attainable and will probably become commonplace.

The computer age has definitely found its way into the lipid analytical laboratory. For some needs, such as laboratories that only perform a few separations a week, the more modest systems, such as strip chart recorders or integrators, may still be the best option. However, for laboratories that perform numerous lipid analyses per week, the recent advances in chromatography data systems have enabled the lipid analyst to electronically store vast quantities of chromatographic data, to recall it any time, and to manipulate the data into many types of reports, including publication quality laser-printed figures. For the reader who would like other perspectives on this topic, two other review articles on chromatography data systems are available (3,4). For the lipid analyst who is contemplating the purchase of a new chromatographic data system and is unsure about what type of system is most appropriate for his/her needs, a recent publication may help to evaluate specific needs (5).

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